

## Intramolecular force fields and vibrational amplitudes of some octahedral systems<sup>‡</sup>

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The MOVFF, MUBFF and GVFF force fields are employed to compute the force constants for some octahedral systems viz.,  $A_2BI^7+O_6$  ( $A = Ba^{2+}, Sr^{2+}$ ,  $B = Li^+, Na^+, K^+$ ),  $ZrF_6^{2-}$ ,  $WF_6$ ,  $[Cr(NH_3)_6]^{3+}$ ,  $[Co(NH_3)_6]^{3+}$  and  $[Ni(NH_3)_6]^{2+}$  using current vibrational data. Moreover, mean amplitudes for these systems have also been computed at temperatures:  $T = 0^\circ K, 298.15^\circ K$  and  $500^\circ K$  along with Coriolis coupling constants. The results are used to study the influence of cations on the relative stability of the chemical bonds in the present systems as well as in the isoelectronic series. The results have been found to be in good agreement with the values reported in literature.

### 1. INTRODUCTION

In recent years, modified version of the conventional force fields have played an important role in understanding the intramolecular forces in octahedral systems. However, modified orbital valence force field (MOVFF) and modified Urey-Bradley force field (MUBFF) involving six and seven parameters have not been thoroughly investigated. In order to examine their usefulness in understanding the stability of the chemical bonds in different environments, the MOVFF, MUBFF and GVFF force fields have been employed to compute the force constants. In addition, the mean amplitudes of vibration and Coriolis constants for  $F_{1u} \times F_{1u}$  type have also been calculated. The octahedral systems under present study include  $10_6^{5-}$  in four different environments (viz.,  $Ba_2Li^{5+}$ ,  $Ba_2Na^{5+}$ ,  $Ba_2K^{5+}$  and  $Sr_2Na^{5+}$ ),  $ZrF_6^{2-}$ ,  $WF_6$ ,  $[Cr(NH_3)_6]^{3+}$ ,  $[Co(NH_3)_6]^{3+}$  and  $[Ni(NH_3)_6]^{2+}$ . The vibrational spectra of these systems have recently been studied by De Hair *et al* (1974) ( $10_6^{5-}$ ), Toth & Bates (1974) ( $ZrF_6^{2-}$ ), McDowell and Asprey (1973) ( $WF_6$ ), Schmidt & Müller (1974) [ $[Cr(NH_3)_6]^{3+}$  and  $[Co(NH_3)_6]^{3+}$ ] and Müller *et al* (1974) [ $[Ni(NH_3)_6]^{2+}$ ]. The observed vibrational frequencies have been interpreted assuming octahedral symmetry. The computed results are used to study the stability of the chemical bonds in different environments and in the isoelectronic series.

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## 2 METHOD OF COMPUTATION

The systems possessing octahedral symmetry give rise to six fundamental vibrations which are distributed among different species as follows—

$$\sqrt{\text{vib}} = \nu_1(a_{1g}) + \nu_2(e_g) + \nu_3(f_{1u}) + \nu_4(f_{1u}) + \nu_5(f_{2u}) + \nu_6(f_{2u}).$$

Among these vibrations  $\nu_1(a_{1g})$ ,  $\nu_2(e_g)$  and  $\nu_5(f_{2g})$  are Raman active,  $\nu_3(f_{1u})$  and  $\nu_4(f_{1u})$  are infrared active while  $\nu_6(f_{2u})$  is inactive in both. The inactive  $\nu_6(f_{2u})$  is permitted as binary combination bands or can be computed with the help of the relation  $\nu_6 = \sqrt{2\nu_5}$ . In cases where any particular frequency has not been reported, we have borrowed it from similar systems (De Hair *et al* 1974).

Wilson's (1955) FG matrix method was employed to calculate the force constants in the MOVFF, MUBFF and GVFF models. The mean amplitudes of vibration were evaluated at temperatures  $T = 0^\circ\text{K}$ ,  $298.15^\circ\text{K}$  and  $500^\circ\text{K}$  using Cyvin's secular equation (1968),  $|\Sigma G^{-1} - \Delta E| = 0$ , where the symbols have their usual meanings.  $F$  and  $G$  matrix elements and the analytical expression for mean amplitudes of vibration were taken from literature [Cyvin (1968), Ramaswamy & Muthusubramaniam (1971), Sanyal *et al* (1974)]. The two dimensional equations occurring in  $f_{1u}$  species were solved by Muller's  $L$ -matrix method [Müller & Peacock (1968), Müller (1968) and Peacock & Müller (1968)]. The  $UCC$  have been evaluated by following Meal & Polo (1956). The molecular constants have been calculated for the skeletons of hexamine metal complexes using point mass model.

## 4. RESULTS AND DISCUSSION

The table 1 presents the vibrational frequencies used in the present computation.

The tables 2-4 list the results of the computed force constants employing MOVFF, MUBFF and GVFF force fields respectively. The results of mean amplitudes of vibration are presented in table 6.

The MOVFF and MUBFF employ bond stretching force constant  $K$ , angle bending force constant  $D(H)$  and interaction constants  $F$ ,  $F'$ ,  $k$ ,  $h$  and  $g$ . The GVFF model includes  $f_r$  bond stretching constant,  $f_u$  angle bending constant and the following interaction constants  $f_{rr}$  and  $f'_{rr}$  which represent cis- and trans-bond stretching interactions respectively,  $f_{\alpha\alpha}$ ,  $f'_{\alpha\alpha}$ ,  $f''_{\alpha\alpha}$  and  $f'''_{\alpha\alpha}$  angle bending interactions. The force constants in GVFF and mean amplitudes, computed by other workers have also been included in the tables 4 and 6 respectively for comparison. It is obvious from the tables that values are in good agreement with those reported earlier.

Table 1. Fundamental vibrational wave-numbers (in  $\text{cm}^{-1}$ ) of octahedral systems

System	$\nu_1(a_{1g})$	$\nu_2(e_g)$	$\nu_3(f_{1u})$	$\nu_4(f_{1u})$	$\nu_5(f_{2g})$	$\nu_6(f_{2u})$	Reference
$\text{Ba}_2\text{LiIO}_6$	694	600	653	423	434	306.88*	De Hair <i>et al</i> (1974)
$\text{Ba}_2\text{NaIO}_6$	722	600 <sup>1</sup>	688	427	435	307.59*	De Hair <i>et al</i> (1974)
$\text{Ba}_2\text{KIO}_6$	702	600 <sup>1</sup>	664	417	434	306.88*	De Hair <i>et al</i> (1974)
$\text{Sr}_2\text{NaIO}_6$	736	658	696	433	461	325.98*	De Hair <i>et al</i> (1974)
$\text{ZrF}_6^{2-}$	585	580	529	217	277	195	Toth & Bates (1974)
$\text{WF}_6(v_1)^a$	772 $\pm$ 1	678 $\pm$ 1	713 $\pm$ 1	252 $\pm$ 1	320 $\pm$ 1	129 $\pm$ 2	McDowell & Asprey (1973)
$\text{WF}_6(\omega_1)^b$	791 $\pm$ 12	693 $\pm$ 8	733 $\pm$ 7	253 $\pm$ 8	330 $\pm$ 10	136 $\pm$ 13	McDowell & Asprey (1973)
$[\text{C}(\text{NH}_3)_6]^{3+}$	465	412	471	270	270	206	Schmitt & Müller (1974)
$[\text{Co}(\text{NH}_3)_6]^{3+}$	494	442	477	331	322	227.7*	Schmitt & Müller (1974)
$[\text{Ni}(\text{NH}_3)_6]^{2+}$	370	251	334	215	235	168	Müller <i>et al</i> (1974)

<sup>a</sup> Harmonic frequency

<sup>b</sup> Observed frequency

\* computed,

<sup>1</sup> borrowed,

Table 2. MOVFT constants (in mdyne/Å)

System	<i>K</i>	<i>D</i>	<i>F</i>	<i>F'</i>	<i>k</i>	<i>h</i>
Ba <sub>2</sub> LiIO <sub>6</sub>	2.621	0.697	0.444	0.062	0.144	0.157
Ba <sub>2</sub> NaIO <sub>6</sub>	2.846	0.579	0.505	-0.002	0.049	0.095
Ba <sub>2</sub> KIO <sub>6</sub>	2.627	0.651	0.472	0.055	0.128	0.145
Sr <sub>2</sub> NaIO <sub>6</sub>	2.912	0.847	0.484	0.143	0.256	0.236
ZrF <sub>6</sub> <sup>2-</sup>	2.305	0.408	0.223	0.202	0.633	0.204
WF <sub>6</sub> (ν <sub>T</sub> ) <sup>a</sup>	4.242	-0.100	0.518	0.010	0.356	0.118
WF <sub>6</sub> (ω <sub>1</sub> ) <sup>b</sup>	4.411	-0.120	0.562	0.019	0.345	0.127
[Cr(NH <sub>3</sub> ) <sub>6</sub> ] <sup>3+</sup>	1.163	0.277	0.223	0.068	0.112	0.072
[Co(NH <sub>3</sub> ) <sub>6</sub> ] <sup>3+</sup>	1.209	0.434	0.204	0.102	0.183	0.140
[Ni(NH <sub>3</sub> ) <sub>6</sub> ] <sup>2+</sup>	0.431	0.043	0.236	-0.011	-0.001	0.008

a—Observed frequency, b—Harmonic frequency

Table 3. MUBFT constants (in mdyne/Å)

System	<i>K</i>	<i>H</i>	<i>F</i>	<i>F'</i>	<i>k</i>	<i>h</i>	<i>g</i>
Ba <sub>2</sub> LiIO <sub>6</sub>	3.082	0.331	0.312	0.070	0.260	0.004	0.639
Ba <sub>2</sub> NaIO <sub>6</sub>	3.288	0.276	0.377	-0.130	0.119	-0.023	0.042
Na <sub>2</sub> KIO <sub>6</sub>	3.142	0.305	0.326	-0.091	0.198	-0.010	0.035
Sr <sub>2</sub> NaIO <sub>6</sub>	3.578	0.395	0.298	-0.044	0.337	0.010	0.032
ZrF <sub>6</sub> <sup>2-</sup>	2.833	0.179	0.060	0.038	0.759	0.007	-0.013
WF <sub>6</sub> (ν <sub>T</sub> ) <sup>a</sup>	5.019	-0.075	0.300	-0.209	0.453	-0.062	-0.054
WF <sub>6</sub> (ω <sub>1</sub> ) <sup>b</sup>	5.284	-0.086	0.317	-0.226	0.451	-0.072	-0.060
[Cr(NH <sub>3</sub> ) <sub>6</sub> ] <sup>3+</sup>	1.342	0.131	0.159	0.003	0.193	-0.001	0.013
[Co(NH <sub>3</sub> ) <sub>6</sub> ] <sup>3+</sup>	1.405	0.207	0.198	0.035	0.253	0.032	0.014
[Ni(NH <sub>3</sub> ) <sub>6</sub> ] <sup>2+</sup>	0.634	0.006	0.173	-0.075	0.049	-0.035	-0.005

a—Observed frequency, b—Harmonic frequency

In order to study the influence of cations on the relative stability of the chemical bonds, it is useful to see the trend in the bond stretching force constants. The regular variation in the force constant *K* observed for periodates (Pavoz Ahmed *et al* 1974) is not observed in the case of perovskites here. A comparison of the bond stretching force constant *K* from the table 2 shows that *K* is smaller for Ba<sub>2</sub>LiIO<sub>6</sub> than Ba<sub>2</sub>NaIO<sub>6</sub>. The trend in perovskites can be explained as follows. In the ordered perovskite structure of the compounds,

Table 4. GYFF constants (in  $\text{mdyn}/\text{\AA}$ )

System	$f_r$	$f_{rr}$	$f_s$	$f_{rs}-f''_{rs}$	$f_x-f''_{xx}$	$f_{xz}-f''_{xz}$	$f_{zz}-f''_{zz}$
$\text{Ba}_2\text{LiIO}_6$	3.566	0.191	0.209	0.121	0.523	0.039	0.039
$\text{Ba}_2\text{NaIO}_6$	3.781	0.253	0.119	0.123	0.529	0.042	0.042
$\text{Ba}_2\text{KIO}_6$	3.612	0.209	0.198	0.118	0.514	0.035	0.035
$\text{S}_2\text{NaIO}_6$	4.086	0.171	0.337	0.127	0.565	0.032	0.032
$\text{ZrFe}_2^d$	3.028 (3.123) <sup>c</sup>	0.011 (0.177) <sup>c</sup>	0.750 (0.677) <sup>c</sup>	0.049	0.189 (0.205) <sup>c</sup>	-0.012 (0.004) <sup>c</sup>	-0.013
$\text{WF}_6(\nu_1)^a$	5.200 (5.23) <sup>d</sup>	0.254 (0.25) <sup>d</sup>	0.543 (0.42) <sup>d</sup>	0.045 (0.09) <sup>d</sup>	0.179 (0.18) <sup>d</sup>	0.043 (0.045) <sup>d</sup>	-0.054 (-0.055) <sup>d</sup>
$\text{WF}_6(\omega)^b$	5.467 (5.50±0.07) <sup>d</sup>	0.271 (0.27±0.04) <sup>d</sup>	0.451 (0.42±0.07) <sup>d</sup>	0.046 (0.094±0.02) <sup>d</sup>	0.185 (0.186) <sup>d</sup>	0.041 (0.041) <sup>d</sup>	-0.060 (-0.059) <sup>d</sup>
$[\text{Co}(\text{NH}_3)_6]^{3+}$	1.666 (1.723) <sup>*</sup> (1.720) <sup>c</sup>	0.078 (0.078) <sup>*</sup> (0.080) <sup>c</sup>	0.193 (0.133) <sup>*</sup> (0.130) <sup>c</sup>	0.081 (0.130) <sup>*</sup>	0.209 (0.210) <sup>*</sup>	-0.002 (0.000) <sup>*</sup>	0.013 (0.020) <sup>*</sup>
$[\text{Co}(\text{NH}_3)_6]^{3-}$	1.870 (1.952) <sup>*</sup> (1.950) <sup>c</sup>	0.081 (0.082) <sup>*</sup> (0.080) <sup>c</sup>	0.253 (0.172) <sup>*</sup> (0.170) <sup>c</sup>	0.116 (0.275) <sup>*</sup>	0.289 (0.345) <sup>*</sup>	0.014 (0.043) <sup>*</sup>	0.014 (0.043) <sup>*</sup>
$[\text{Ni}(\text{NH}_3)_6]^{2-}$	0.830 (0.86) <sup>f</sup>	0.124 (0.12) <sup>f</sup>	0.049 (0.04) <sup>f</sup>	0.049 (0.08) <sup>f</sup>	0.130 (0.14) <sup>f</sup>	0.002 (0.00) <sup>f</sup>	-0.005 (0.00) <sup>f</sup>

a-Observed frequency. b-Harmonic frequency. c-Values from Toth and Bates (1974). d-Values from McDowell and Asprey (1973). e-Values from Schmidt and Müller (1974). f-Values from Müller *et al.* (1974). \*Calculated from given values of symmetrised constants in Schmidt and Müller (1974).

every oxygen is joined linearly by one monovalent cation and one  $I^{7+}$  ion. Since the ionic radius of  $Li^+$  is smaller than the  $Na^+$  ion therefore  $Li^+$  ion weakens the  $I^{7+}-O^{2-}$  bond more than the  $Na^+$  ion and this effect is translated in stretching force constant. On similar grounds we should expect an even higher value of  $K$  in case of  $Ba_2KIO_6$  because  $K^+$  has larger ionic radius but this trend is not followed. It may be due to the indication of the broadening of lines and bands in the spectra of these compounds and some amount of disorder of the  $Ba^{2+}$  and  $K^+$  ions whose radii are  $1.35\text{\AA}$  and  $1.33\text{\AA}$  respectively, because nearly equal ionic radii of  $Ba^{2+}$  and  $K^+$  also tend to distort the structure which under ideal conditions will have 12 coordination sites for  $Ba^{2+}$  and 6 for  $K^+$ . The larger  $K$  value for  $Sr_2NaIO_6$  than  $Ba_2NaIO_6$  can be understood in terms of cell dimensions.  $Sr^{2+}$  has smaller ionic radius than  $Ba^{2+}$  and the cell constant of  $Sr_2NaIO_6$  ( $8.20\text{\AA}$ ) (De Hair *et al* 1974) is also smaller than  $Ba_2NaIO_6$  ( $8.33\text{\AA}$ ) (De Hair *et al* 1974). On account of these two differences, I-O distance is smaller in  $Sr_2NaIO_6$  than in  $Ba_2NaIO_6$  which increases the value of  $K$ . Similar observations have been made by De Hair *et al* (1974) on the basis of simple UBFF studies. The stretching force constants in MUBFF and GVFF (tables 3 and 4 respectively) also follow the similar trend. The bending and interaction force constants in three models do not show regular trend with the change in the ionic radius of the monovalent cation and some constants are also almost equal therefore these have not been discussed.

It is interesting to study the relative stability of the chemical bonds in iso-electronic series. For this purpose we have three sets of isoelectronic series viz. (i)  $-IO_6^{5-}$  (3.76) and  $TeO_6^{6-}$  (4.12) (Pandey *et al* 1973), (ii)  $ZrF_6^{2-}$  (3.03),  $NbF_6^-$  (3.70) (Sharma *et al.* 1974) and  $MoF_6$  (4.79) (LaBonville 1972), and (iii)  $-TaF_6^-$  (3.62) (Pandey *et al* 1973) and  $WF_6$  (5.20) where the values in parentheses are the stretching bond force constants (GVFF) in  $\text{mdyn/\AA}$ . From a comparison of these values, it is found that in case of octahedral, VI oxidation state is more stable than the VII oxidation state, while in case of hexafluoroanions higher oxidation state is more stable. The stability of higher oxidation state in case of hexahalogenous have been reported in literature (LaBonville 1972). The ionic radii of the central atoms and bonded distances in case of hexafluoroanions also support this trend.

A comparison of stretching force constants of  $IO_6^{5-}$  and  $ZrF_6^{2-}$  with their respective di- and tri-oxides and fluorides viz.  $I(VII)O_6^{5-}$  ( $d^0$  3.76)  $I(V)O_3^-$  ( $d^{10} 8^2$  5.10) (Parvez Ahmed *et al* 1974) and  $Zr(IV)F_6^{2-}$  ( $d^0$  3.028),  $Zr(III)F_3$  ( $d^1$  4.16) (Hango *et al* 1973),  $Zr(II)F_2$  ( $d^2$  3.54) (Hango *et al* 1973), (the values in parentheses are stretching force constants in  $\text{mdyn/\AA}$  and number of non-bonding electrons of the central atoms) shows that lower oxidation state to be associated with a higher force constant. In case of fluorides, the crystal field stabilisation energies for configurations,  $d^0 = 0 Dq$ ,  $d^1 = 5 Dq$  and  $d^2 = 6 Dq$  also support the above conclusions except in case of  $ZrF_2$ .

A comparison of stretching force constant  $K$  ( $f_r$ ) (Tables 2, 3 & 4) among hexammine complexes of bivalent and trivalent first row transition metals shows that the strength of the metal ligand bond varies in the order  $\text{Co-N} > \text{Cr-N} > \text{Ni-N}$ . The stability of the chemical bonds can also be understood in terms of 10  $Dq$  values for metal ions and ligand group. The values (Figgis 1966) are 24, 22 and 11 respectively in units of  $\text{cm}^{-1} \times 10^{-3}$  for the configuration  $\text{Co}^{3+}$ ,  $\text{Cr}^{3+}$  and  $\text{Ni}^{2+}$  which are in accordance with the calculated values of force constants.

Coriolis coupling constant (C.C.C) are presented in table 5. Figure 1 represents the variation of  $\xi_{33}$  ( $f_{12}$ ) with the ratio of masses ( $m_r/m_l$ ) of the central and ligand atoms which is in agreement with the trend reported by Müller (1968).

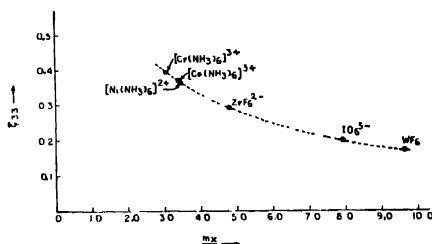


Fig. 1 Variation of Coriolis coupling constant  $\xi_{33}$  with the mass ratio ( $m_r/m_l$ ) of central and ligand atoms.

The mean amplitudes of vibration for bonded as well as for non-bonded distances listed in the table 6 at temperatures;  $T = 0^\circ\text{K}$ ,  $T = 298.15^\circ\text{K}$  and  $T = 500^\circ\text{K}$  show usual variation. It is also noted that the mean amplitude values for the bonded distances show opposite trend than the corresponding stretching force constants as expected. From the comparison of the mean amplitude

Table 5 Coriolis coupling constants of octahedral systems

System	Coriolis coupling constants		$m_r/m_l$
	$\xi_{33}$	$\xi_{41}$	
$\text{IO}_6^{2-}$	0.201	0.290	7.932
$\text{ZrF}_6^{2-}$	0.294	0.206	4.801
$\text{WF}_6$	0.171	0.329	9.677
$[\text{Cr}(\text{NH}_3)_6]^{3+}$	0.304	0.106	3.053
$[\text{Co}(\text{NH}_3)_6]^{3+}$	0.367	0.133	3.460
$[\text{Ni}(\text{NH}_3)_6]^{2+}$	0.369	0.131	3.447

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values in case of isoelectronic series bonded distances at room temperature viz. (i)  $\text{IO}_6^{5-}$  (0.0442 Å),  $\text{TeO}_6^{6-}$  (0.0433 Å) (Pandey *et al* 1973), (ii)  $\text{ZrF}_6^{2-}$  (0.0474),  $\text{NbF}_6^-$  (0.0437 Å) (Sharma *et al* 1974),  $\text{MoF}_6$  (0.0400 Å) (Cyvin 1968) and (iii)  $\text{TaF}_6^-$

Table 6 Mean amplitudes of vibration ( $\text{m}$  Å)

System		0°K	290.15°K	500°K
$\text{Ba}_2\text{LiIO}_6$	X-Y	0.0429	0.0410	0.0503
	Y-Y <sub>short</sub>	0.0720	0.0806	0.0944
	Y-Y <sub>long</sub>	0.0579	0.0608	0.0681
$\text{B}_{12}\text{NaIO}_6$	X-Y	0.0423	0.0441	0.0492
	Y-Y <sub>short</sub>	0.0714	0.0797	0.0932
	Y-Y <sub>long</sub>	0.0576	0.0604	0.0679
$\text{Ba}_2\text{KIO}_6$	X-Y	0.0428	0.0447	0.0500
	Y-Y <sub>short</sub>	0.0720	0.0806	0.0944
	Y-Y <sub>long</sub>	0.0578	0.0607	0.0683
$\text{Sr}_2\text{NaIO}_6$	X-Y	0.0415	0.0430	0.0476
	Y-Y <sub>short</sub>	0.0701	0.0775	0.0901
	Y-Y <sub>long</sub>	0.0556	0.0577	0.0641
$\text{ZrF}_6^{2-}$	X-Y	0.0442	0.0474	0.0545
	Y-Y <sub>short</sub>	0.0843	0.1091	0.1340
	Y-Y <sub>long</sub>	0.0552	0.0587	0.0668
$\text{WF}_6(\nu_1)^a$	X-Y	0.0371	0.0384 (0.038 ± 0.003)* (0.0383)**	0.0423
	Y-Y <sub>short</sub>	0.0769	0.1084 (0.101 ± 0.005)* (0.104)**	0.1345
	Y-Y <sub>long</sub>	0.0501	0.0518 (0.065 ± 0.011)* (0.0516)**	0.0572
$\text{WF}_6(\omega_1)^b$	X-Y	0.0367	0.0378 (0.0377 ± 0.0004)**	0.0415
	Y-Y <sub>short</sub>	0.0758	0.1050 (0.100 ± 0.005)**	0.1290
	Y-Y <sub>long</sub>	0.0495	0.0511 (0.0509 ± 0.0003)**	0.0562
$[\text{Cr}(\text{NH}_3)_6]^{3+}$	X-Y	0.0538	0.0603	0.0711
	Y-Y <sub>short</sub>	0.0958	0.1194	0.1458
	Y-Y <sub>long</sub>	0.0680	0.0773	0.0919
$[\text{Co}(\text{NH}_3)_6]^{3+}$	X-Y	0.0521	0.0579	0.0680
	Y-Y <sub>short</sub>	0.0896	0.1072	0.1296
	Y-Y <sub>long</sub>	0.0657	0.0735	0.0866
$[\text{Ni}(\text{NH}_3)_6]^{2+}$	X-Y	0.0640	0.0810	0.0998
	Y-Y <sub>short</sub>	0.1077	0.1470	0.1835
	Y-Y <sub>long</sub>	0.0839	0.1105	0.1373

a—Observed frequency, b—Harmonic frequency,

\*—Experimental from Seip & Seip (1966), \*\*—from Mc Dowell & Asprey (1973).



(0.0436 Å) (Sharma *et al* 1974),  $WF_a$  (0.0385 Å) (Cyvin 1968) (values in parentheses are mean amplitudes), it is found that they show opposite trend than the corresponding stretching force constants. From this it is concluded that in case of hexafluoroanions stronger bonds have smaller mean amplitudes. Similar trend has also been noted in literature.

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